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A Systematic Methodology for Uncertainty Analysis of Group Contribution Based and Atom Connectivity Index Based Models for Estimation of Properties of Pure Components

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One of the most widely employed group contribution method for estimation of properties of pure components is the Marrero and Gani (MG) method. For the given component whose molecular structure is not completely described by any of the available groups, group contribution⁺ method (combined MG method and atomic connectivity index method) has been employed to create the missing groups and predict their contributions through the regressed contributions of connectivity indices. The objective of this work is to develop a systematic methodology to carry out uncertainty analysis of group contribution based and atom connectivity index based property prediction models. This includes: (i) parameter estimation using available MG based property prediction models and large training sets to determine improved group and atom contributions; and (ii) uncertainty analysis to establish statistical information such as covariance, standard error and confidence intervals. The developed methodology allows estimation of following properties: normal boiling point, critical constants, standard enthalpy of formation, standard enthalpy of vaporization, standard Gibbs energy, normal melting point, standard enthalpy of fusion, entropy of vaporization, surface tension, viscosity, flash point, auto ignition temperature, Hansen solubility parameters, Hildebrand solubility parameter, aqueous solubility, octanol/water partition coefficient, compressibility factor, molar volume, molar refraction, refractive index and lethal concentration. The application of the developed methodology is highlighted through a set of molecules not used in the parameter estimation step. The developed methodology can be used to assist uncertainty and sensitivity analysis of product/process design to obtain rationally the risk/ safety factors and to provide confidence in the obtained process calculations.